CONTENTS

Physical properties of metal–hydrogen systems: some new aspects related to the electronic and atomic structure 1
J. P. Burger (Orsay, France)

The influence of hydrogenation on the magnetic properties and hyperfine interactions of amorphous Fe–Zr alloys 17
S. M. Fries (Saarbrücken, F.R.G.), C. L. Chien (Baltimore, MD, U.S.A.), J. Crummenauer, H.-G. Wagner and U. Gonser (Saarbrücken, F.R.G.)

Magnetic, crystallographic and hydrogen absorption properties of YMn_2 and $ZrMn_2$ hydrides 25
H. Fujii, M. Saga and T. Okamoto (Hiroshima, Japan)

Recent magnetic studies of complex metal hydrides 33
W. E. Wallace, F. Pourarian, A. T. Pedziwiatr and E. B. Boltich (Pittsburgh, PA, U.S.A.)

Effect of nickel, gadolinium and lanthanum substitution on the magnetic properties of Y_2Co_7 hydride 47
M. Yamaguchi, T. Ohta (Yokohama, Japan), T. Goto, T. Sakakibara (Tokyo, Japan) and T. Katayama (Ibaraki, Japan)

Magnetic properties of NdH_{2+x} compounds 55
S. Senoussi, J. N. Daou, P. Vajda and J. P. Burger (Orsay, France)

Absorption of hydrogen in ultrathin palladium and palladium-based alloys 61
M. Nicolas, H. Raffy, L. Dumoulin and J. P. Burger (Orsay, France)

Comparison of structures and electronic properties between $TiCoH_x$ and $TiFeH_x$ 69
J. S. Cantrell (Oxford, OH, U.S.A.) and R. C. Bowman, Jr. (Los Angeles, CA, U.S.A.)

Electrical resistance and hydrogen solubility anomalies in a Pd–8at.%Y solid solution alloy 79
M. Doyle, R. C. J. Wileman and I. R. Harris (Birmingham, U.K.)

Effects of rhombohedral distortion on the magnetic properties of $REFe_2$ hydrides (Re = Er, Tb) 89
D. Fruchart (Grenoble, France), Y. Berthier, T. De Saxe (Saint-Martin-d'Hères, France) and P. Vuillet (Grenoble, France)

Hydrogen induced changes of valency and hybridization in cerium intermetallic compounds 97
D. Fruchart, F. Vaillant, A. Yanouanc, J. M. D. Coey (Grenoble, France), R. Fruchart, Ph. L'Héritier (St. Martin d'Hères, France), T. Riesterer, J. Osterwalder and L. Schlapbach (Zürich, Switzerland)

Proton nuclear magnetic resonance in the ferromagnetic hydride $EuLiH_3$ 105
K. Kojima, T. Imai, K. Hiraoka and T. Hihara (Hiroshima, Japan)

Thermodynamic, structural and magnetic properties of $LaNi_{5-x}Fe_x$ hydrides 111
J. Lamloumi (Tunis, Tunisia), A. Percheron-Guégan, C. Lartigue, J. C. Achard (Meudon, France) and G. Jehanno (Gif-sur-Yvette, France)

Electron–phonon coupling and superconductivity of hydrogen implanted aluminium 123
X. W. Lin and M. Gupta (Orsay, France)

In situ electron microscopy study of implanted AlH_x 133
X. W. Lin, M. O. Ruault, A. Traverse and H. Bernas (Orsay, France)

Hydriding behaviour of FeTi and $FeTi_{1.15}$: ease of activation and skipping of β region 139
P. Raj, A. Satyamoorthy, P. Suryanarayana, A. J. Singh and R. M. Iyer (Bombay, India)

Coherent phase transition in NbH_x studied by neutron radiography 147
G. Steyrer (Grenoble, France and Munich, F.R.G.) and J. Peisl (Munich, F.R.G.)

γ–γ perturbed angular correlation studies of dysprosium hydrides 155
L. P. Ferreira (Coimbra, Portugal), G. Teisseron, P. Vulliet (Grenoble, France), J. M. Gil, P. J. Mendes, A. P. De Lima and N. Ayres de Campos (Coimbra, Portugal)

Magnetic and electronic properties of Hf_2Fe hydrides. 163
G. Teisseron, P. Vulliet (Grenoble, France) and L. Schlapbach (Zürich, Switzerland)

Mössbauer and time-differential perturbed angular correlation studies of the hydrides and deuterides of vanadium 173
L. Iannarella, M. Baier, M. Zelger and F. E. Wagner (Garching, F.R.G.)

On the breakdown of the iron sublattice long-range magnetic order in RFeAl hydrides (R ≡ rare earth) 181
G. Wiesinger (Vienna, Austria)

Proton magnetic resonance in the paramagnetic state of GdH_3 187
O. J. Żogał (Wrocław, Poland)

^{51}V nuclear magnetic resonance and magnetic susceptibility study of the electronic structure in Ti–V dihydrides 193
B. Nowak (Wrocław, Poland), Y. Chabre and R. Andreani (Saint-Martin-d'Hères, France)

*Magnetoresistance and magnetic susceptibility of hydrides of disordered Ni–Mn alloys 201
D. K. Schwarz and H. J. Bauer (Munich, F.R.G.)

*Statistical model for the distribution of hydrogen atoms and deuterium atoms around substitutional (interstitial) trapping centres 202
G. Cannelli, R. Cantelli and F. Cordero (Rome, Italy)

*Nature and some consequences of stress-induced states of hydrogen in b.c.c. metals 202
Yuh Fukai, K. Watanabe (Tokyo, Japan) and E. Yagi (Saitama, Japan)

*Neutron vibrational spectroscopy and hydrogen potential of β-V_2H. 203
R. Hempelmann (Jülich, F.R.G.), D. Richter (Grenoble, France) and D. Price (Argonne, IL, U.S.A.)

*Separation of crystal-field levels and phonons in the RE dehydrides using polarized neutrons 204
R. R. Arons (Jülich, F.R.G.), J. W. Cable and R. M. Nicklow (Oak Ridge, TN, U.S.A.)

---

*Abstract or a paper presented at the International Symposium on the Properties and Applications of Metal Hydrides V, Maubuisson, France, May 25 - 30, 1986.

*Magnetic order of the non-stoichiometric light RE dideuterides 205
R. R. Arons, A. Heidel (Jülich, F.R.G.) and J. W. Cable (Oak Ridge, TN, U.S.A.)

*Anelastic relaxation due to the tunnelling of H and D in some transition metal . . . 206
G. Cannelli, R. Cantelli and F. Cordero (Rome, Italy)

*Lattice location study of H in Ta by the channelling method 207
E. Yagi, S. Nakamura, T. Kobayashi, F. Kano (Saitama, Japan), K. Watanabe, Y. Fukai and T. Osaka (Tokyo, Japan)

4. ELECTRONIC STRUCTURE

Electronic rearrangement in the dilute vanadium and niobium hydrides 209
A. Mokrani, C. Demangeat (Strasbourg, France) and G. Moraitis (Antananarivo, Madagascar)

Electronic properties of $LaNi_5$ and $LaNi_5H_7$ 219
M. Gupta (Orsay, France)

Calculations of the electronic structure of disordered transition metal dihydrides 229
D. A. Papaconstantopoulos and P. M. Laufer (Washington, DC, U.S.A.)

Low temperature electronic properties of cerium hydrides 239
L. Schlapbach, H. R. Ott, E. Felder, H. Rudigier (Zürich, Switzerland), P. Thiry, J. Bonnet, Y. Petroff and J. P. Burger (Orsay, France)

Electronic structure and total energy calculations for transition metal hydrides. . . . 249
A. C. Switendick (Albuquerque, NM, U.S.A.)

The calculation of the electronic properties of the monohydride of cobalt by the linear muffin-tin orbital method 261
E. S. Alekseev, N. I. Kulikov and A. F. Tatarchenko (Moscow, U.S.S.R.)

An experimental and theoretical investigation of the densities of states of dimagnesium cobalt pentahydride 267
E. Belin (Paris, France), M. Gupta (Orsay, France), P. Zolliker and K. Yvon (Genève, Switzerland)

Electronic structure of hydrogen in nickel and its trapping by impurities 275
Z. Badirkhan, J. Khalifeh (Amman, Jordan) and C. Demangeat (Strasbourg, France)

Hydrogen in iron, vanadium and FeV: heat of formation, lattice location and the hydrogen–metal bond 285
Ch. Minot (Orsay, France) and C. Demangeat (Strasbourg, France)

Theoretical study of the X-ray absorption spectra of Mg_2FeH_6 293
E. Orgaz and M. Gupta (Orsay, France)

Photoemission study of the electronic structure of Zr–Pd compounds and their relation to hydride formation 301
L. Schlapbach, S. Hüfner, S. Büchler and T. Riesterer (Zürich, Switzerland)

*Effect of hydrogen absorption on the electronic and structural properties of V–Fe alloys 307
A. Ostrasz and E. Debowska (Wrocław, Poland)

*Electronic density of states from pressure–composition isotherms in metal hydrides 307
R. Feenstra and R. Griessen (Amsterdam, The Netherlands)

---

*Abstract of a paper presented at the International Symposium on the Properties and Applications of Metal Hydrides V, Maubuisson, France, May 25 - 30, 1986.

5. THERMODYNAMIC PROPERTIES

Thermodynamics of the $ErFe_2$–H(D) system 309
T. B. Flanagan, J. D. Clewley, N. B. Mason and H. S. Chung (Burlington, VT, U.S.A.)

Ordered phases in niobium hydride: predictions using lattice–gas models. 319
C. K. Hall, C. Soteros, I. MacGillivray (Raleigh, NC, U.S.A.) and A. I. Shirley (Plano, TX, U.S.A.)

On the "imaginary binary hydrides" model 329
I. Jacob (Beer-Sheva, Israel)

Calculation of phase equilibria in hydrogen–metal systems 339
W. A. Oates (Shortland, N.S.W., Australia)

New experiments on and interpretation of hysteresis effects of Pd–D_2 and Pd–H_2 351
E. Wicke and J. Blaurock (Münster, F.R.G.)

A numerical expression for the P–C–T properties of metal hydrides 365
H. Bjurström, S. Suda (Tokyo, Japan) and D. Lewis (Nyköping, Sweden)

Evolution of metal–hydrogen bonds in hydridoaluminates 371
J. C. Bureau, J. P. Bastide, P. Claudy, J. M. Lettoffe and Z. Amri (Villeurbanne, France)

Absorption of hydrogen in Pd–Co and Pd–U alloys 375
R. Feenstra, D. C. de Groot, R. Griessen (Amsterdam, The Netherlands), J. P. Burger (Orsay, France) and A. Menovski (Amsterdam, The Netherlands)

Solubility of protium, deuterium and tritium in palladium–silver alloys at low hydrogen concentrations. 387
R. Lässer (Jülich, F.R.G.) and G. L. Powell (Oak Ridge, TN, U.S.A.)

A study of the decomposition of magnesium hydride by thermal analysis. 395
J. S. Han (Seoul, South Korea), M. Pezat (Bordeaux, France) and Jai-Young Lee (Seoul, South Korea)

Comparison of analytical approximation for hydrogen in b.c.c. metals with Monte Carlo calculations 403
P. Meuffels (Jülich, F.R.G.) and W. A. Oates (Shortland, N.S.W., Australia)

Pressure–composition isotherms of thin PdH_c films 415
E. M. Salomons, R. Feenstra, D. C. de Groot, J. H. Rector and R. Griessen (Amsterdam, The Netherlands)

Thermodynamic studies of hydrides of R_6Fe_{23} (R ≡ Y, Er, Ho, Lu) and R_6Mn_{23} (R ≡ Gd, Dy, Er, Ho) 421
H. K. Smith (Pittsburgh, PA, U.S.A.), J J. Rhyne, K. A. Hardman-Rhyne (Gaithersburg, MD, U.S.A.) and W. E. Wallace (Pittsburgh, PA, U.S.A.)

A re-examination of the neptunium–hydrogen system 431
J. W. Ward, W. Bartscher and J. Rebizant (Karlsruhe, F.R.G.)

Thermodynamic and physical properties of yttrium and some rare earth hydrides 441
A. S. Chernikov, V. I. Savin, V. N. Fadeev, N. A. Landin and L. A. Izhvanov (Moscow, U.S.S.R.)

The phase diagram of the vanadium–tritium system 453
R. Lässer and T. Schober (Jülich, F.R.G.)

*The activation of FeTi for hydrogen absorption: progress and possibilities 459
F. D. Manchester and D. Khatamian (Toronto, Canada)

---

*Abstract of a paper presented at the International Symposium on the Properties and Applications of Metal Hydrides V, Maubuisson, France, May 25 - 30, 1986.

*Hydrogen dynamics in the near surface region of palladium 459
R. H. Stulen, T. E. Felter, G. E. Gdowski and G. D. Kubiak (Livermore, CA, U.S.A.)

*Hydrogen profiling in FeTi 463
D. Khatamian, F. D. Manchester and J. M. Perz (Toronto, Canada)

6. SURFACE EFFECTS

Calculation of hydrogen dissociation pathways on nickel using the embedded atom method 465
S. M. Foiles, M. I. Baskes, C. F. Melius and M. S. Daw (Livermore, CA, U.S.A.)

Theory of hydrogen interaction with metals 475
J. K. Nørskov (Copenhagen, Denmark) and F. Besenbacher (Århus, Denmark)

Modifications near the surface owing to hydrogen cycling of the intermetallics $LaNi_5$ and $LaNi_{5-x}Al_x$ 491
J. E. Bonnet, P. Dantzer, H. Dexpert, J. M. Esteva and R. Karnatak (Orsay, France)

Adsorption and subsequent dissolution of hydrogen in $FeTi_{1.14}O_{0.03}$ 497
T. Hirata (Tokyo, Japan)

Electron binding energies and oxidation behaviour in UNiAl, YNiAl and ZrNiAl . . . 503
I. Jacob, M. Fisher and Z. Hadari (Beer Sheva, Israel)

Conversion electron Mössbauer spectroscopy on surface layers of activated FeTi 511
D. Khatamian, F. D. Manchester and J. M. Daniels (Toronto, Canada)

Surface properties of $LaNi_3Mn_2$ hydrogen storage material 517
C. Lartigue, Yu Xin-Nan, Jiang Zhao Xue and Lin Zhang Da (Beijing, China), A. Percheron-Guégan and J. C. Achard (Meudon, France)

Analysis of hydrogen depth profiles in a Ta–Ti sandwich film by the ^{15}N reaction method 525
M. Pilakouta, A. Neskakis, K. Papastaikoudis, A. A. Katsanos (Attiki, Greece), H. Wenzl and K. H. Klatt (Jülich, F.R.G.)

Surface study on thin layers of oxidized titanium–iron alloys as semiconducting photoelectrodes for the production of hydrogen 529
B. Rupp (Jerusalem, Israel), R. Brener (Haifa, Israel), K. J. Hartig (Wien, Austria) and J. Hauck (Jülich, F.R.G.)

Surface properties on hydrogen storage material TiFeMm 535
Yu Xi-Nan and Lin Zhangda (Beijing, China)

*A new approach to the heat of solution of hydrogen in metals 541
T. Riesterer (Zürich, Switzerland)

*A computer controlled microbalance rig for pressure–composition isotherm measurements 541
M. J. Benham, K. D. Grose and D. K. Ross (Birmingham, U.K.)

*Enthalpies of formation and hydrogenation of $LaNi_{5-x}Co_x$ compounds 542
C. Colinet, A. Pasturel (Saint Martin d'Hères, France), A. Percheron-Guégan and J. C. Achard (Meudon, France)

*Calorimetric determination of the electric field gradient in $TaH(D)_{0.5}$ 542
P. Gutsmiedl, K. Neumaier (Garching, F.R.G.) and H. Wipf (Darmstadt, F.R.G.)

---

*Abstract of a paper presented at the International Symposium on the Properties and Applications of Metal Hydrides V, Maubuisson, France, May 25 - 30, 1986.

*Phase diagrams of some rare earth hydrides. 542
E. Kaldis, M. Tellefsen and R. Bischof (Zürich, Switzerland)

*A clean autoclave system for crystal growth and phase diagram studies (about 2500 bar, 1700 °C) 543
J. Karpinski and E. Kaldis (Zürich, Switzerland)

*Two-phase theory of thermodynamic aspects of palladium hydride 544
J. E. Lowther and P. Anagnostaras (Johannesburg, South Africa)

*Spinodals and catastrophes 544
F. Marsiglio and F. D. Manchester (Toronto, Canada)

*The temperature variation of hydrogen solubility in metals. 545
W. A. Oates (Shortland, N.S.W., Australia), R. Lässer and H. Wenzl (Jülich, F.R.G.)

*Calorimetric investigation of the phase transition exhibited by the hydride of Mg_2Ni 545
M. L. Post and J. J. Murray (Ottawa, Canada)

AUTHOR INDEX 547

SUBJECT INDEX 549

*Abstract of a paper presented at the International Symposium on the Properties and Applications of Metal Hydrides V, Maubuisson, France, May 25 - 30, 1986.